

5#

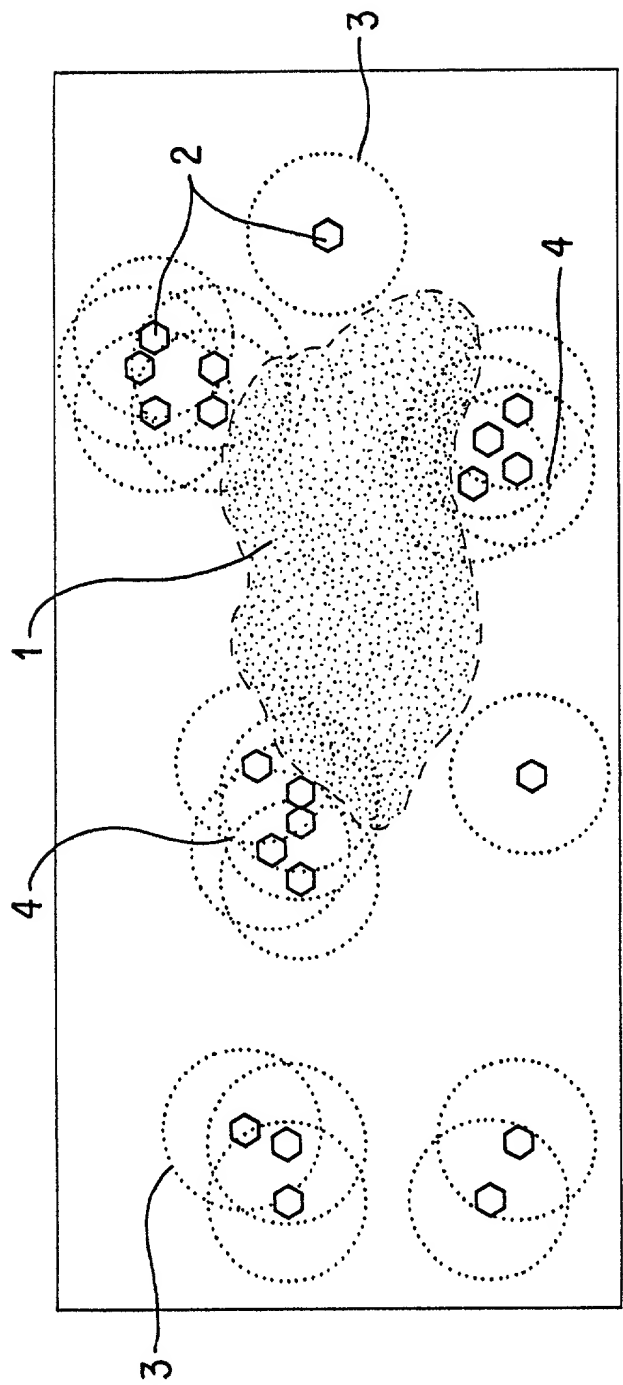


FIG. 1(a)

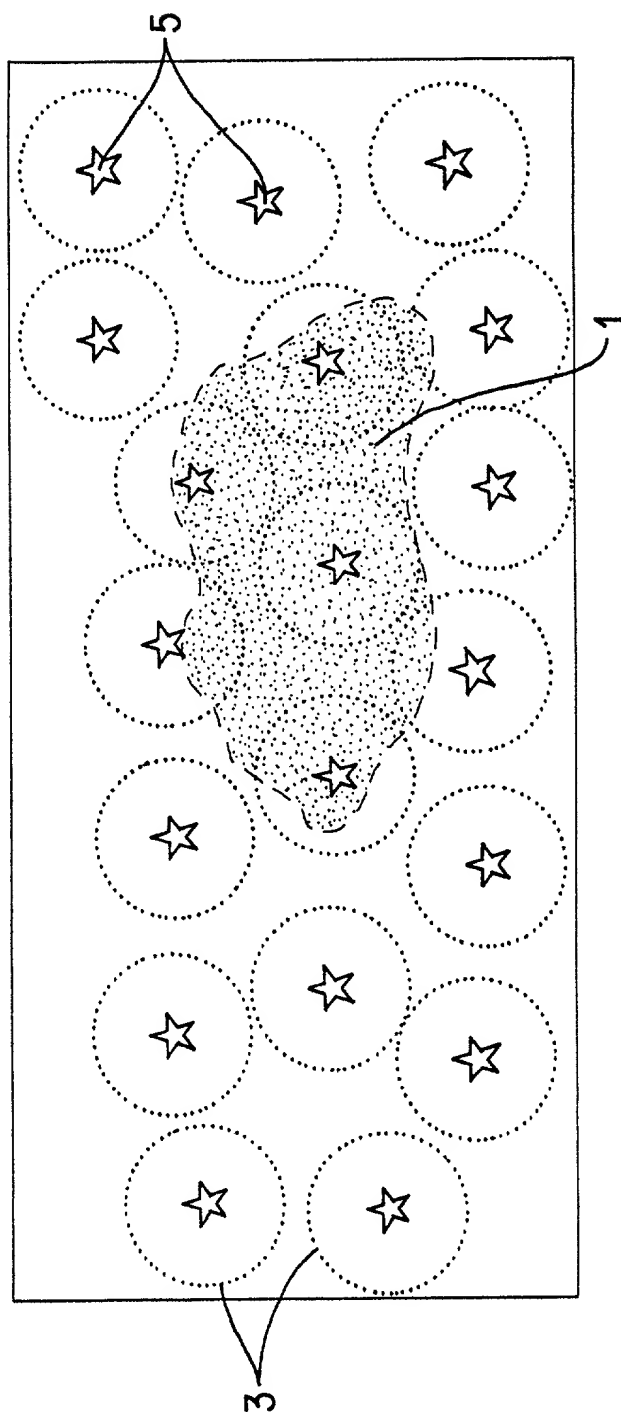


FIG. 1(b)

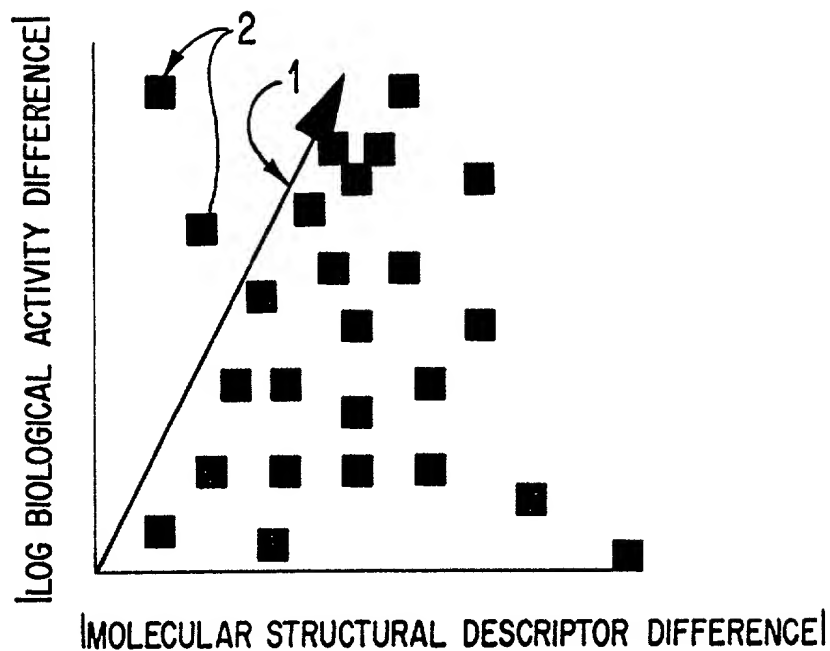


FIG. 2

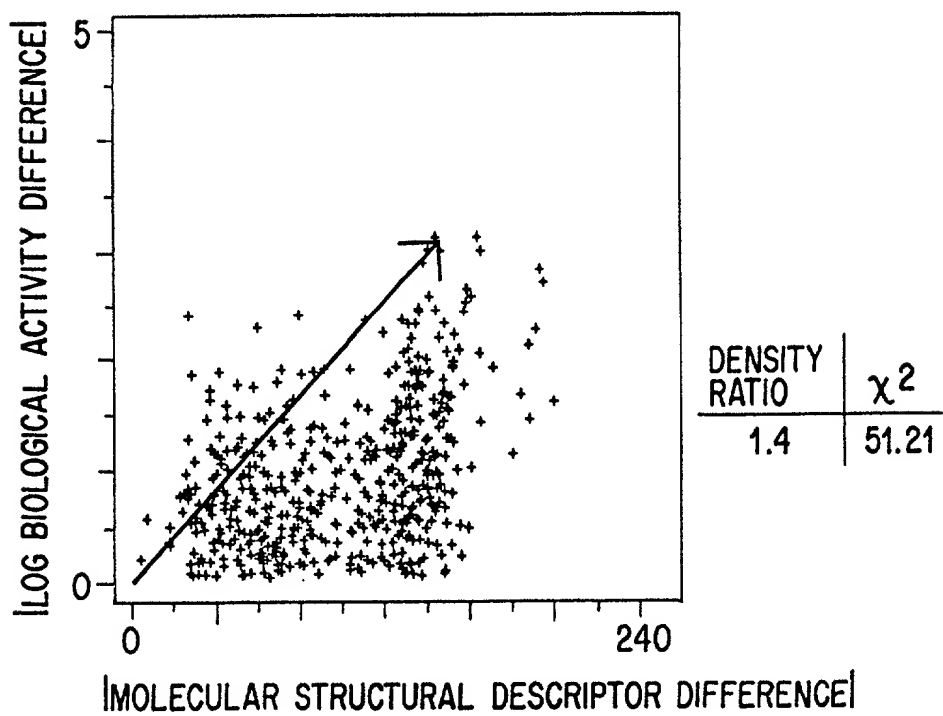


FIG. 3

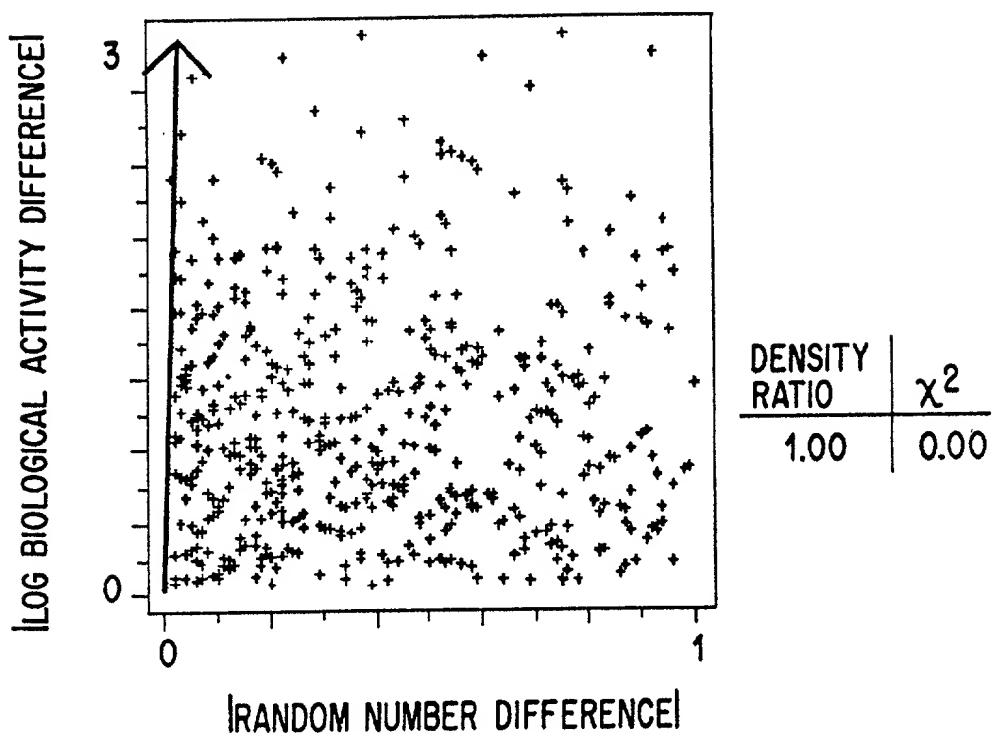


FIG. 4

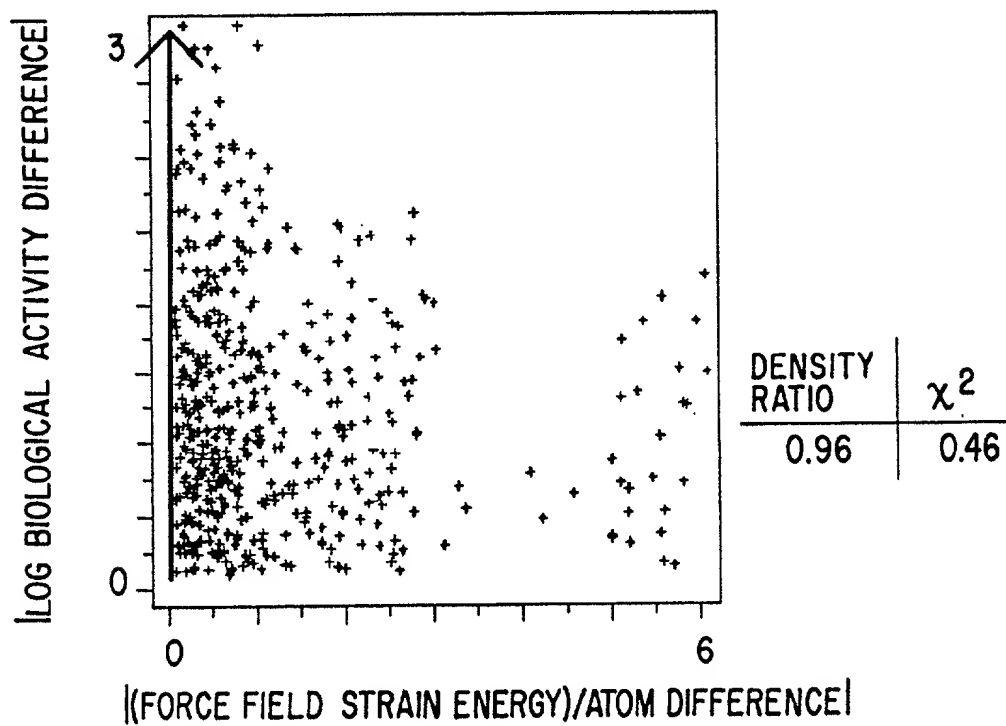
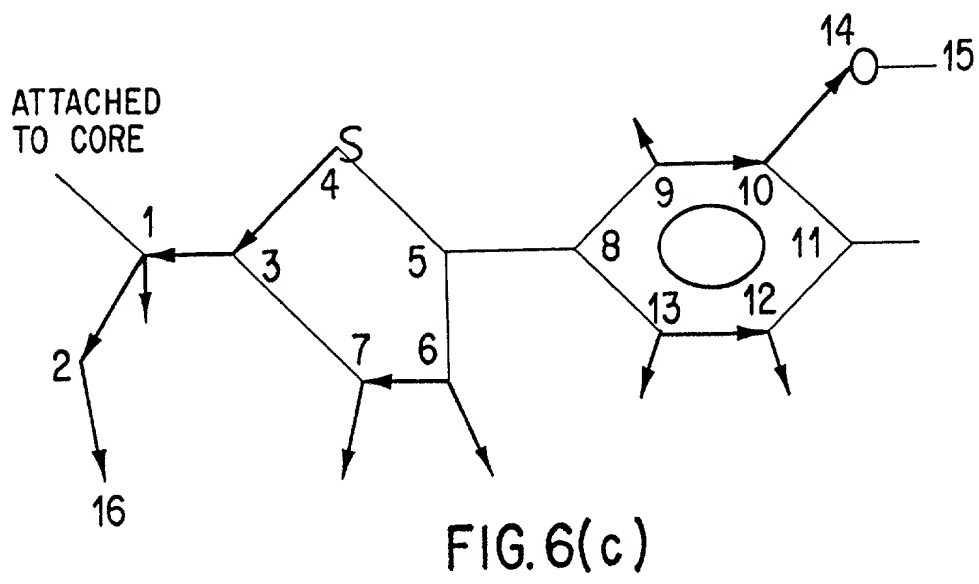
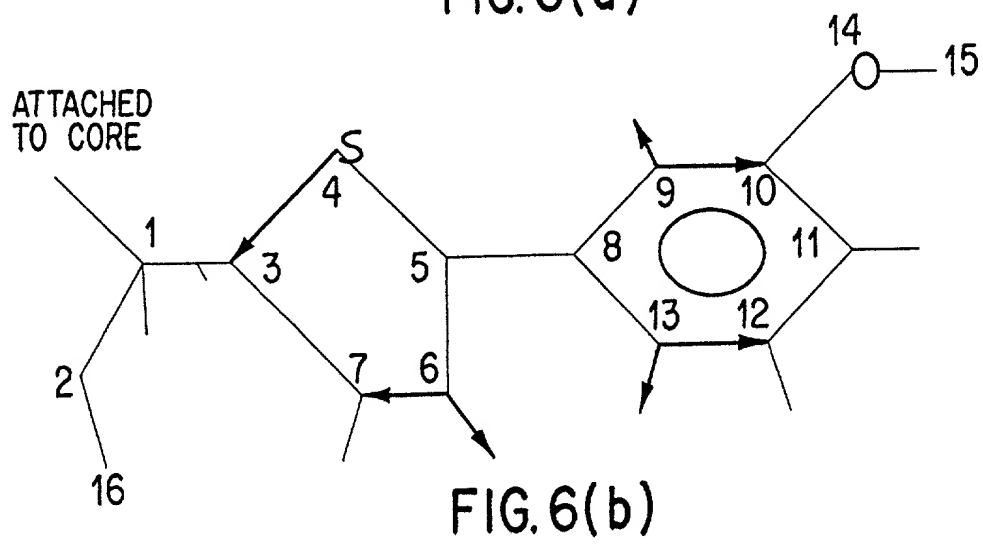
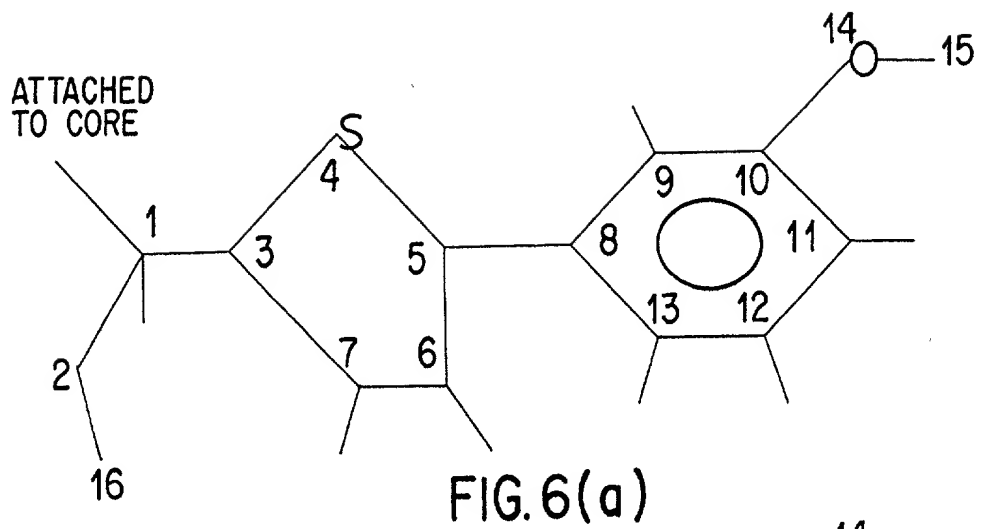


FIG. 5



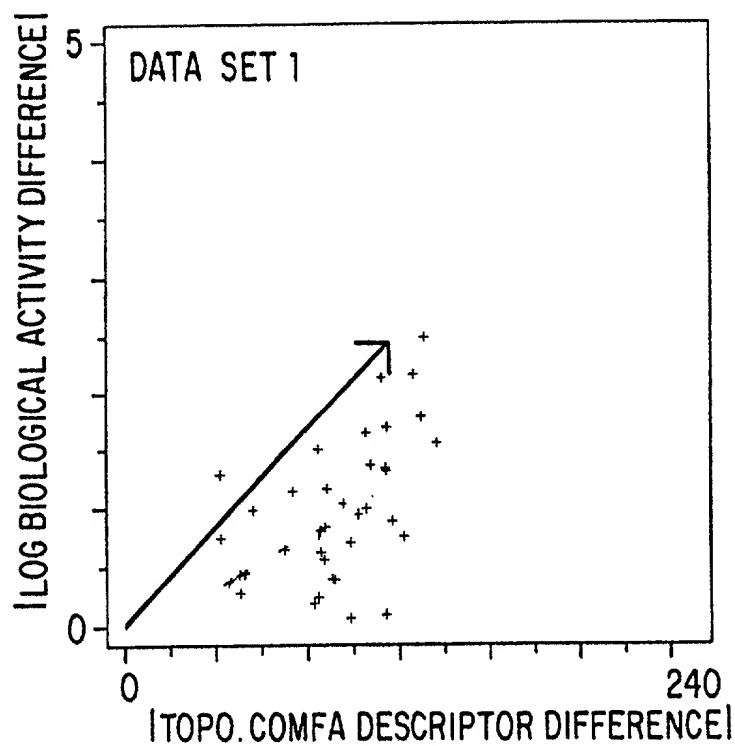


FIG.7(a)

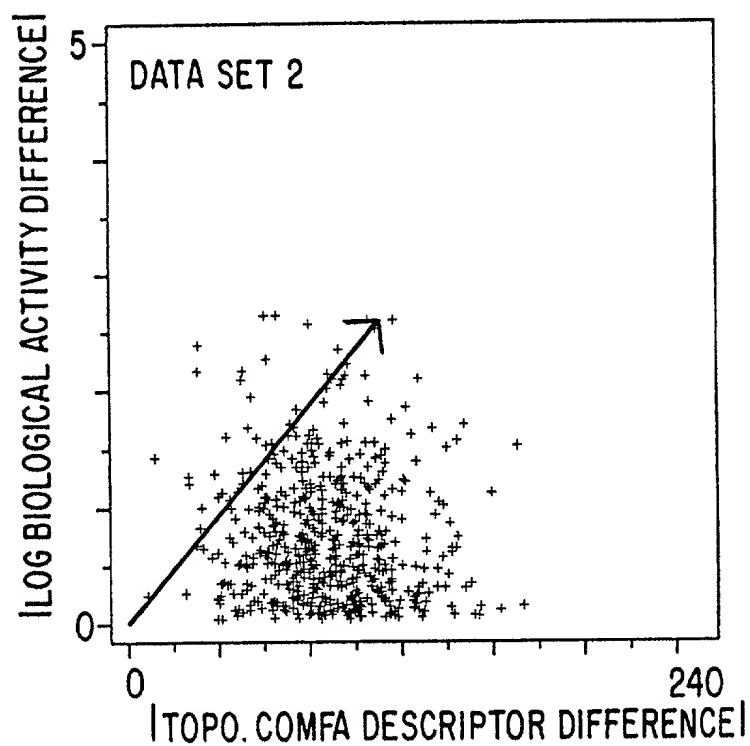


FIG.7(b)

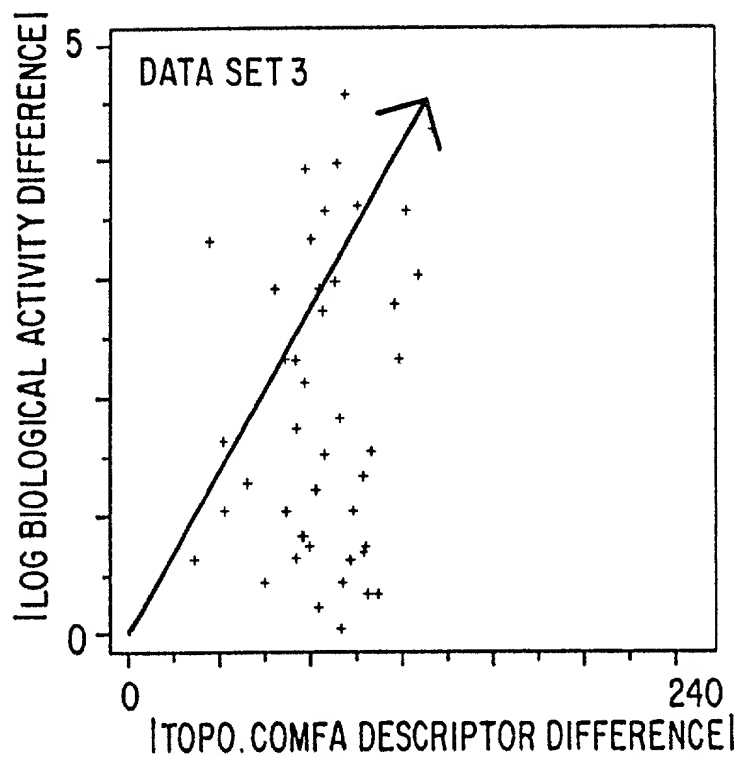


FIG.7(c)

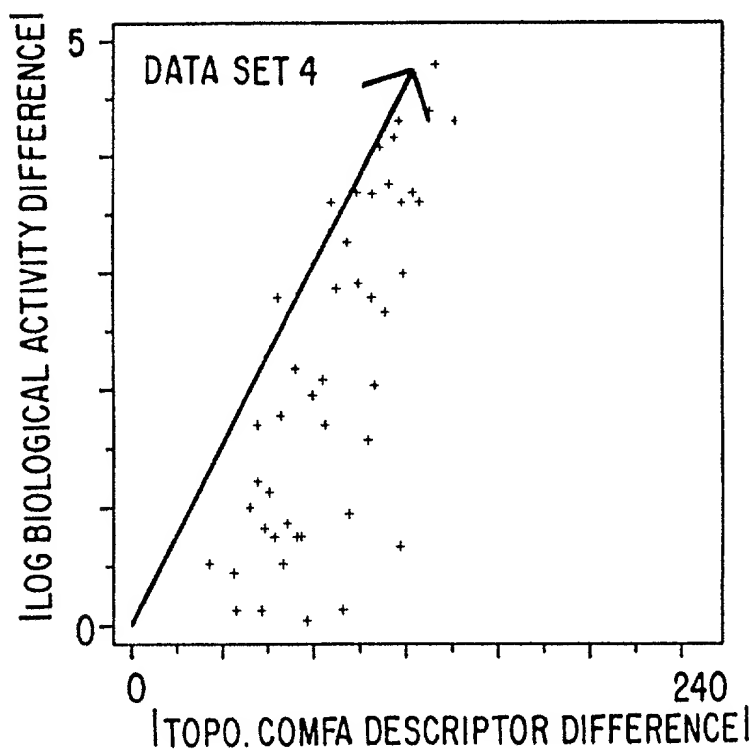


FIG.7(d)

DATA SET 5

Y-axis: |LOG BIOLOGICAL ACTIVITY DIFFERENCE| (0 to 5)

X-axis: |TOPO.COMFA DESCRIPTOR DIFFERENCE| (0 to 240)

DATA SET 6

Y-axis: LOG BIOLOGICAL ACTIVITY DIFFERENCE (0 to 5)

X-axis: |TOPO. COMFA DESCRIPTOR DIFFERENCE| (0 to 240)

FIG. 7(f)



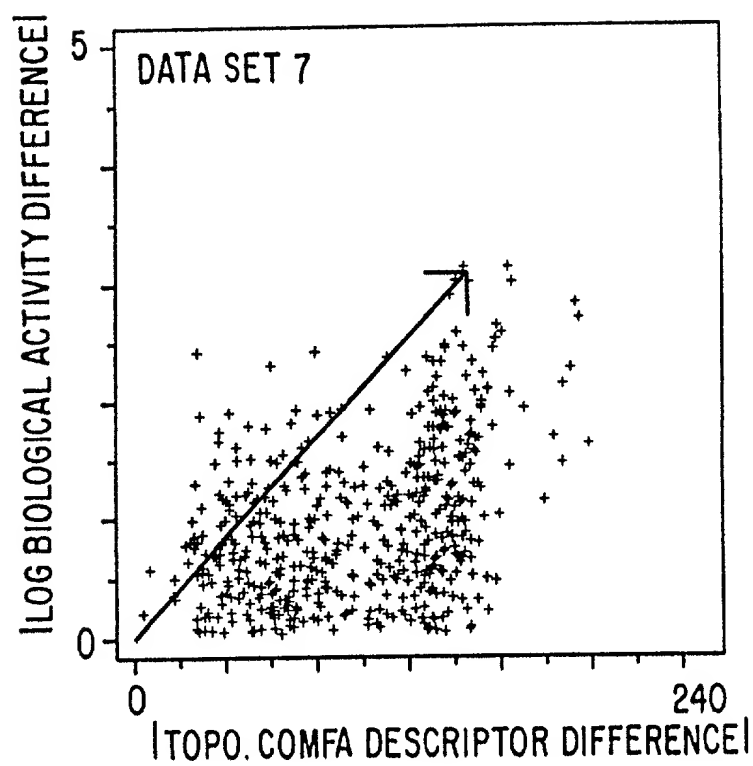


FIG.7(g)

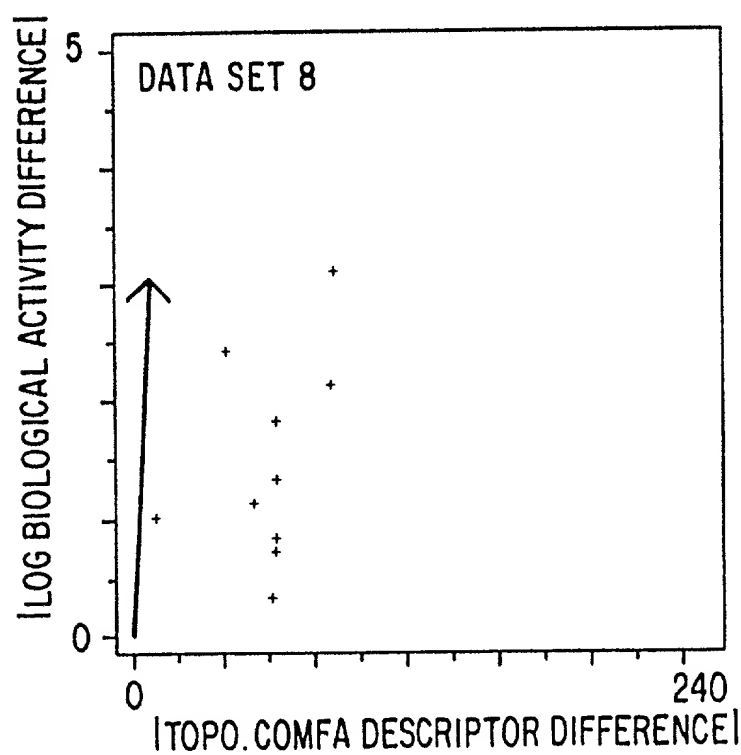


FIG.7(h)

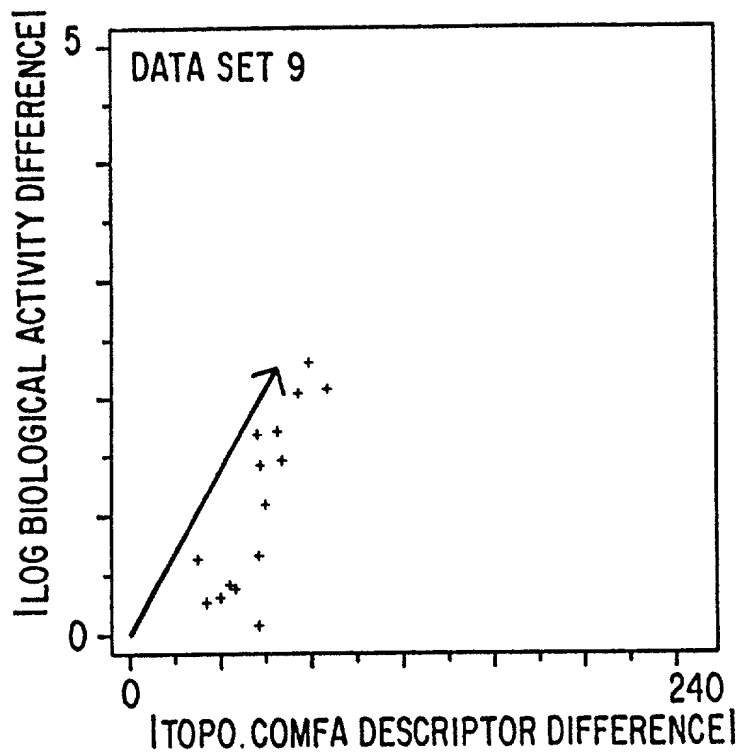


FIG.7(i)

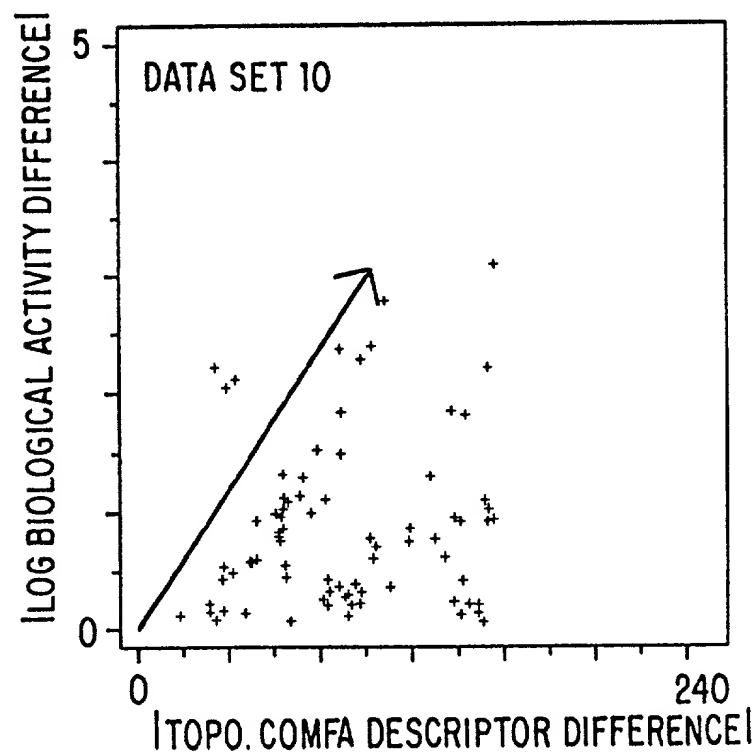


FIG.7(j)

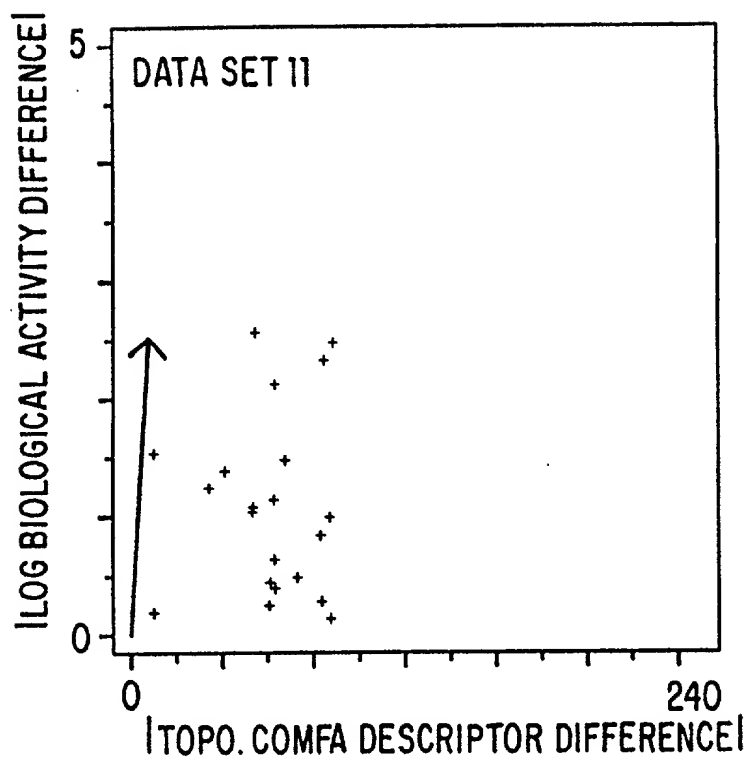


FIG.7(k)

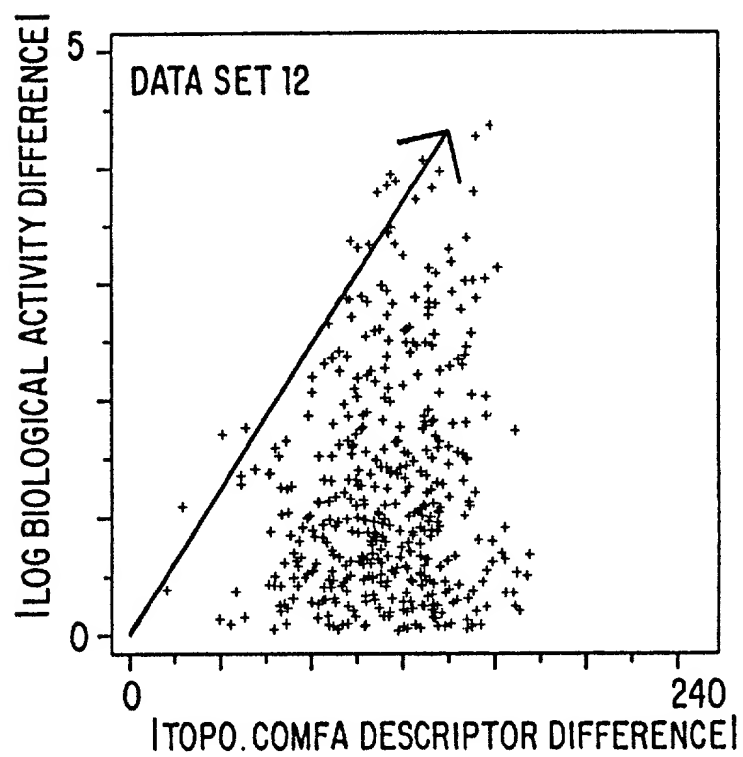


FIG.7(1)

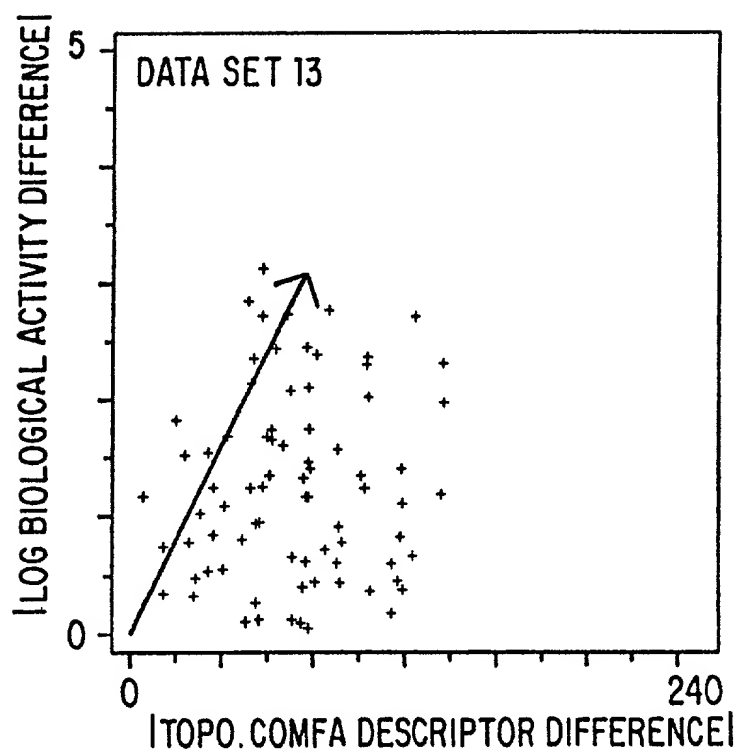


FIG.7(m)

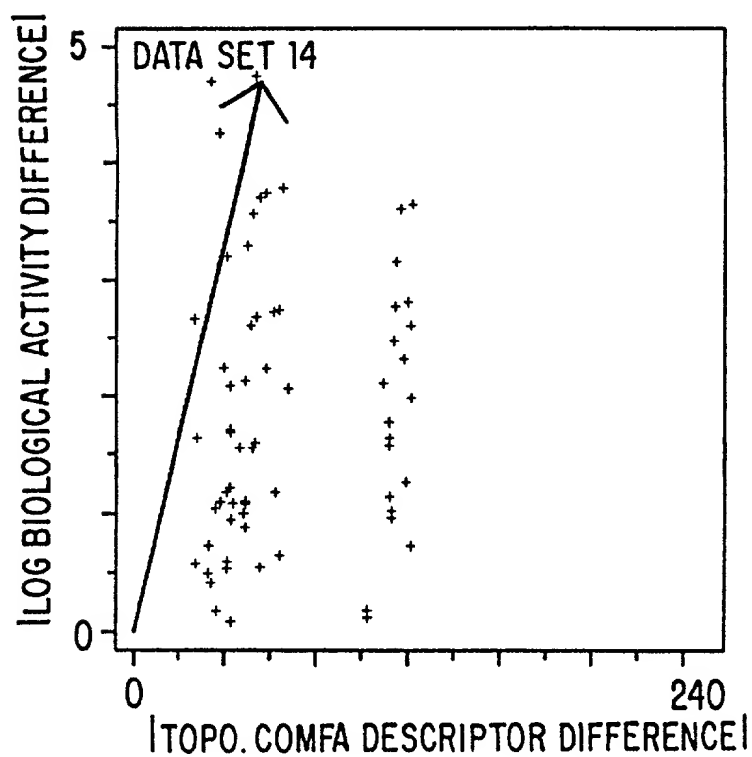


FIG.7(n)

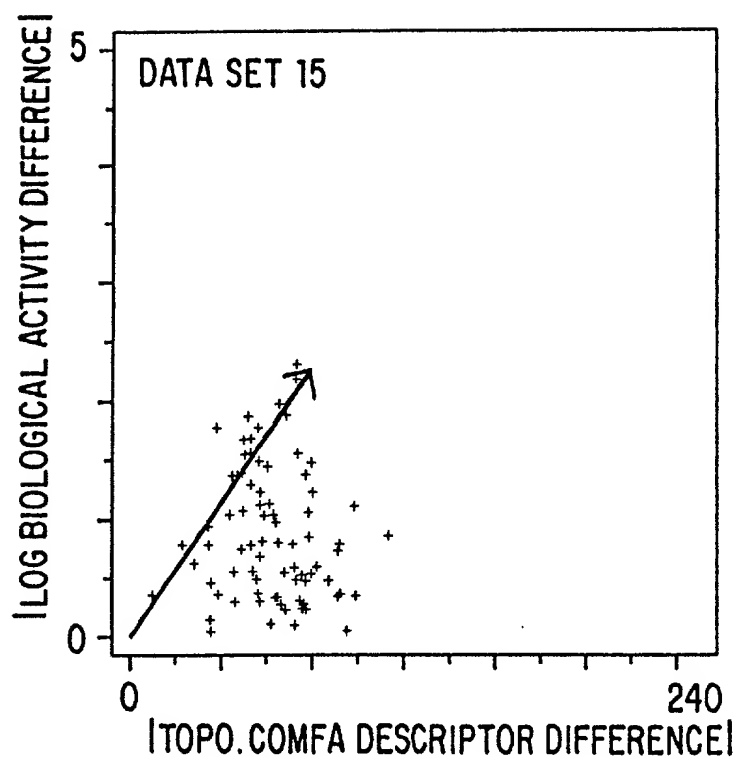


FIG.7(o)

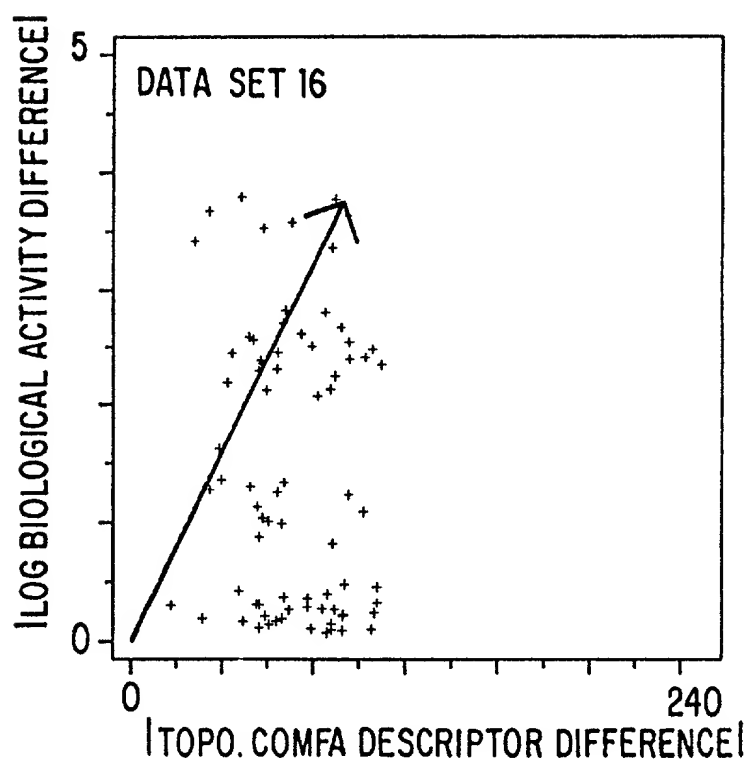


FIG.7(p)

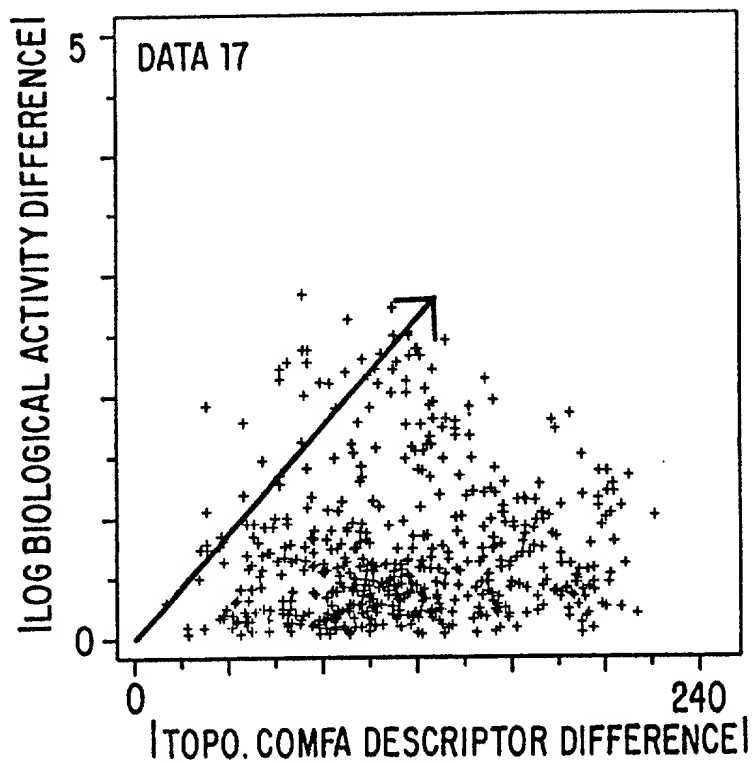


FIG.7(q)

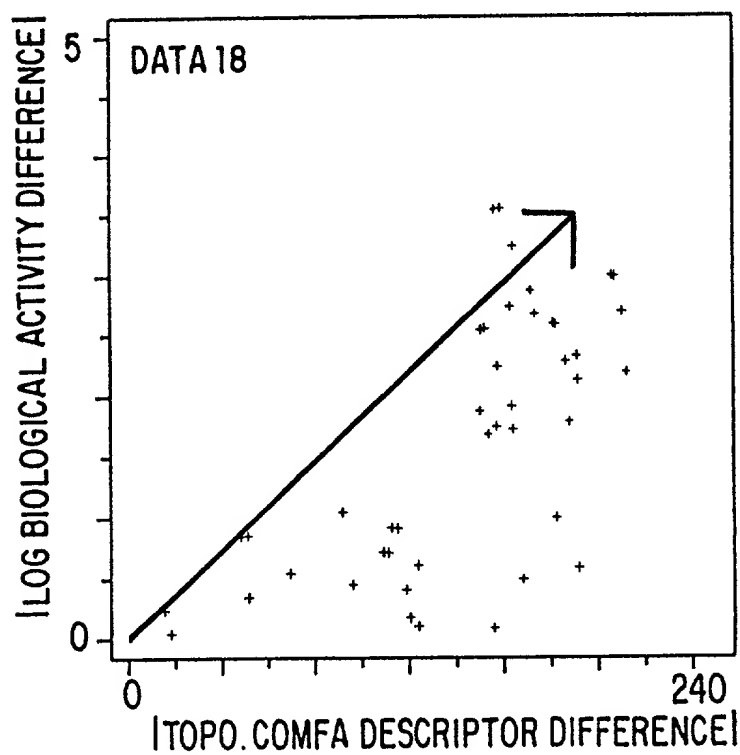


FIG.7(r)

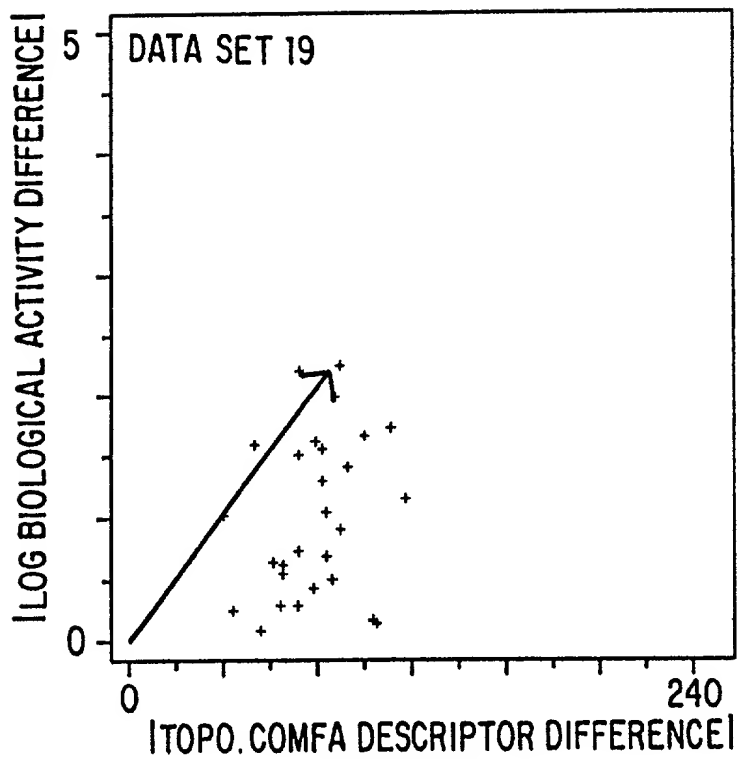


FIG. 7(s)

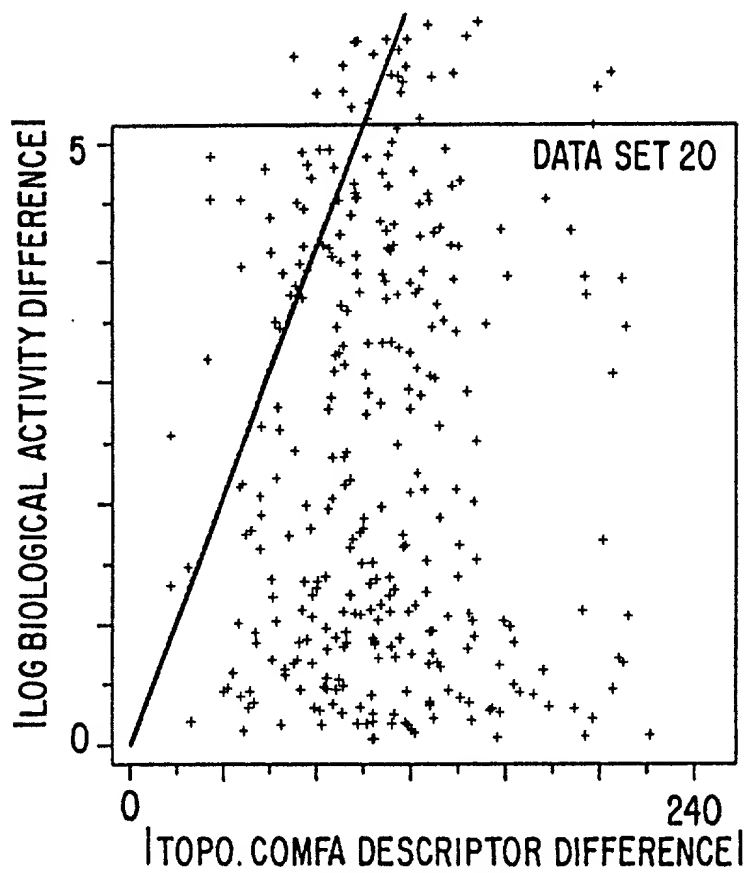
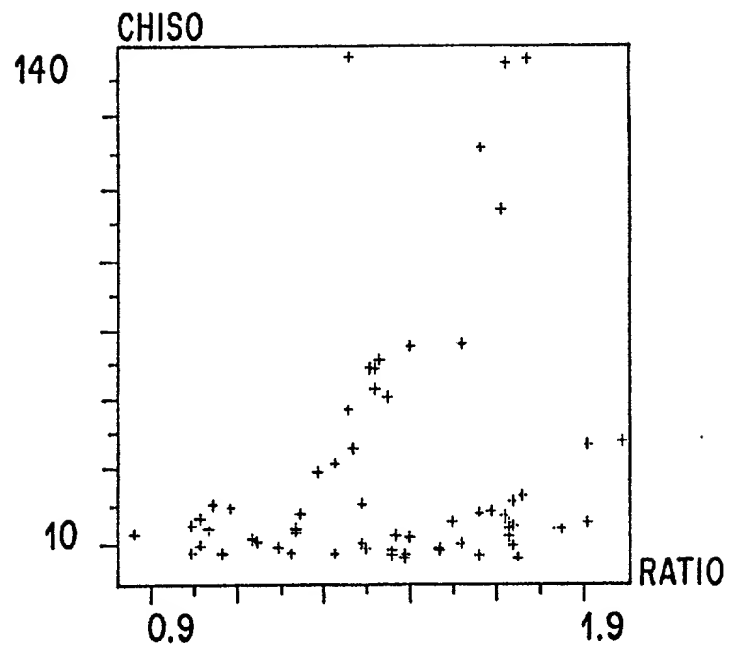
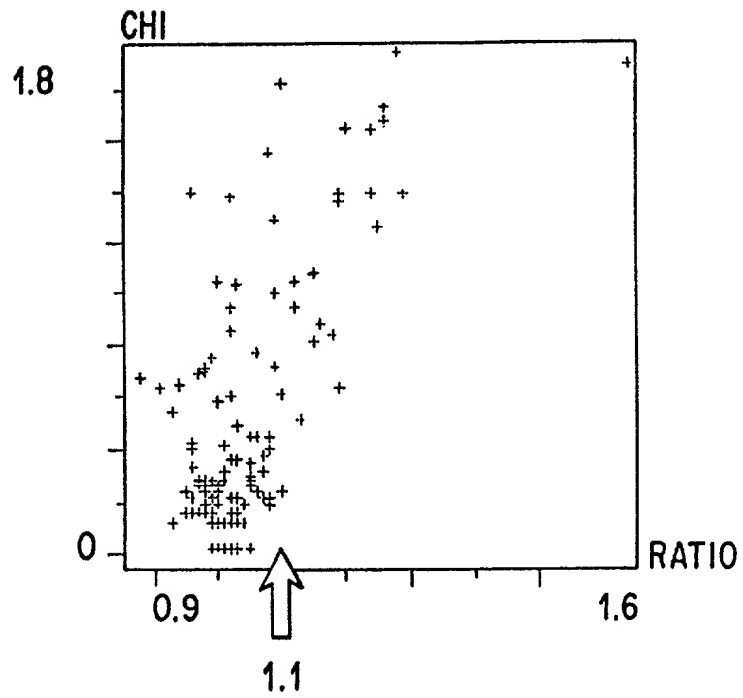


FIG. 7(t)



1.1

FIG. 8(a)



1.1

FIG. 8(b)



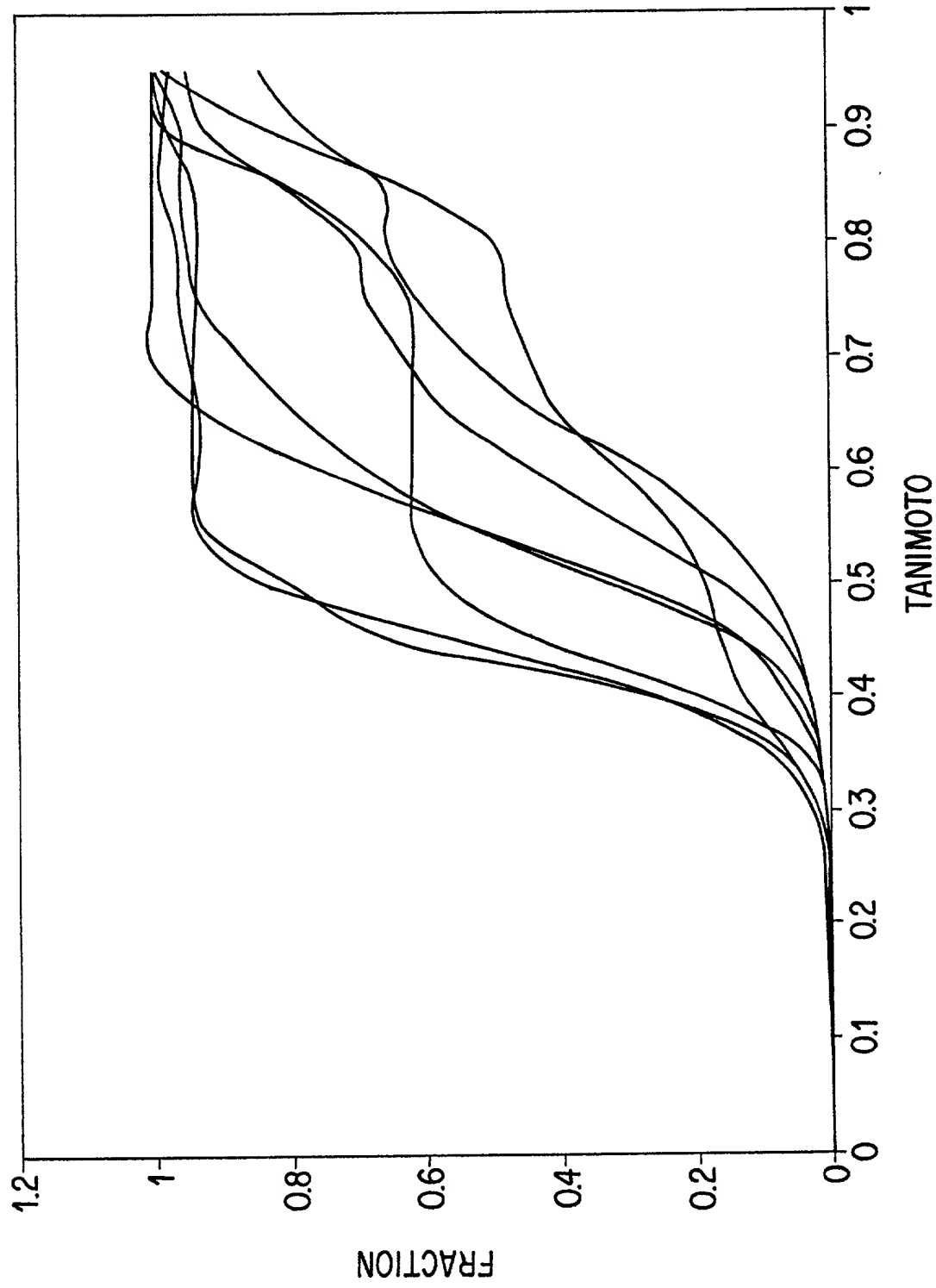


FIG. 9(a)

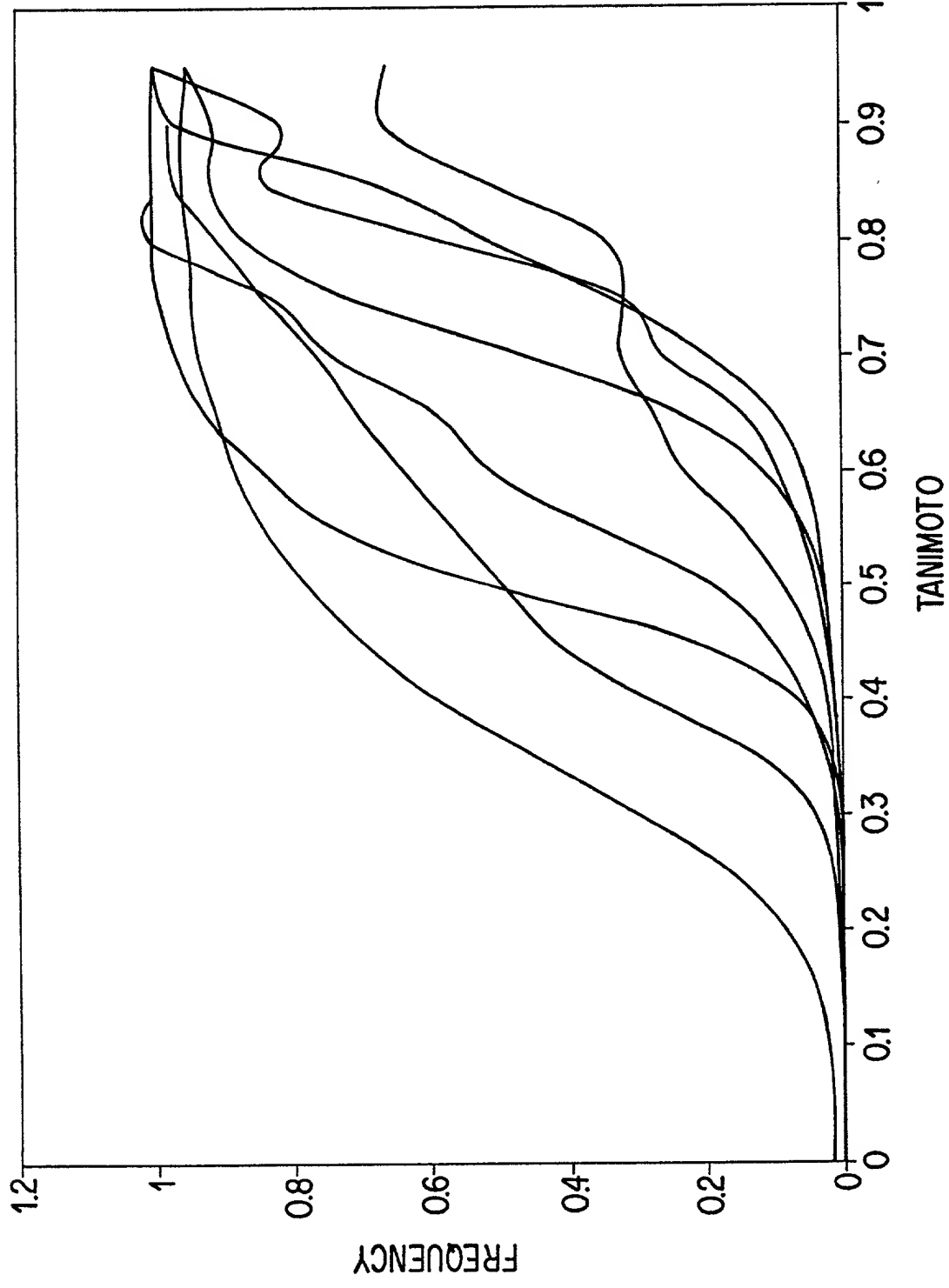
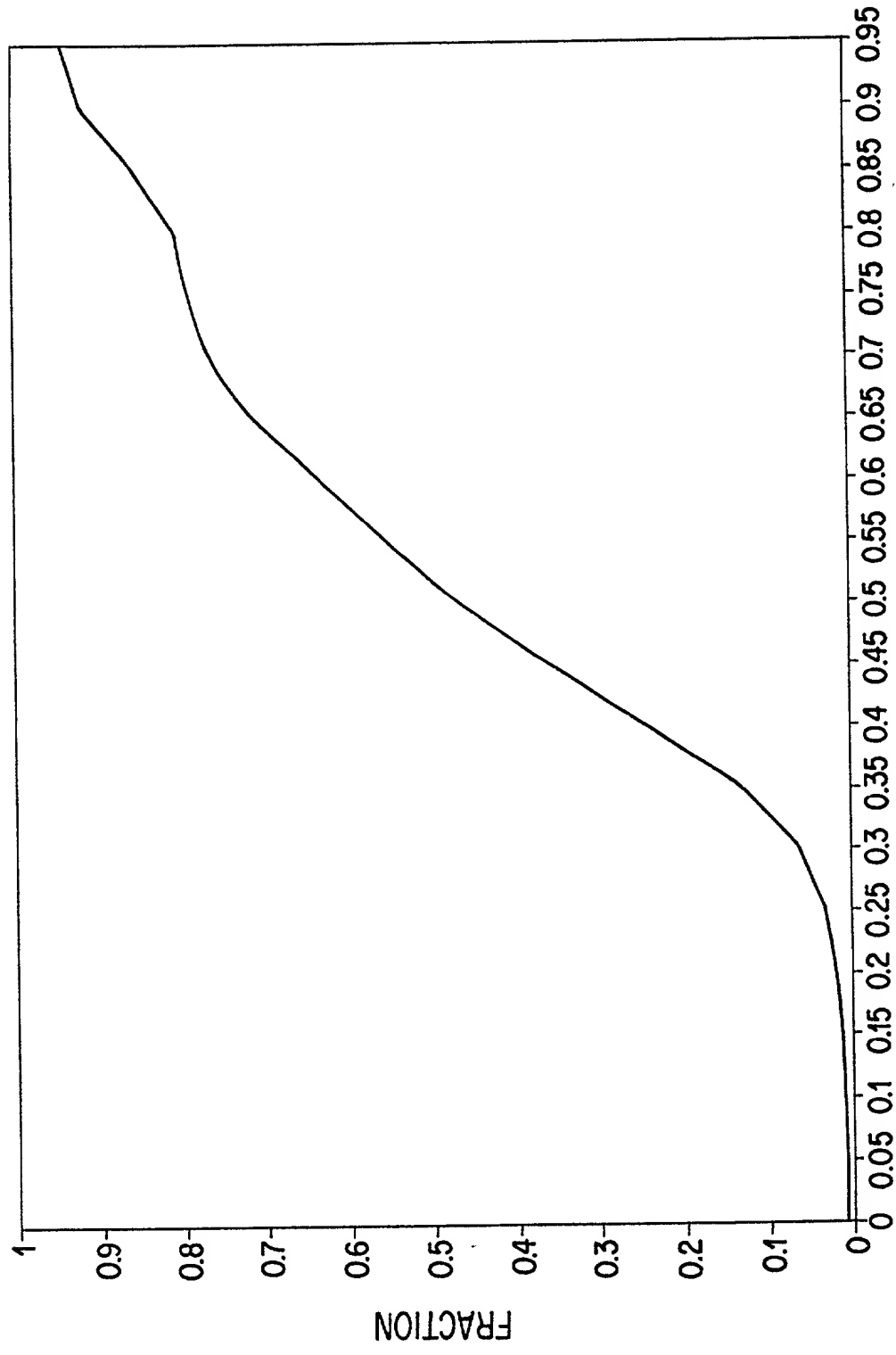


FIG. 9(b)



TANIMOTO

FIG. 9(c)

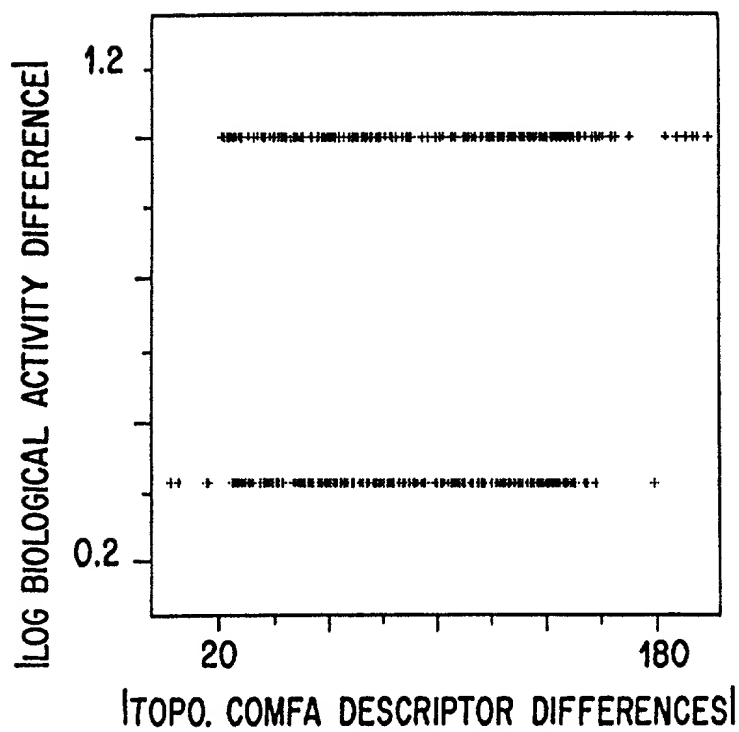


FIG.10(a)

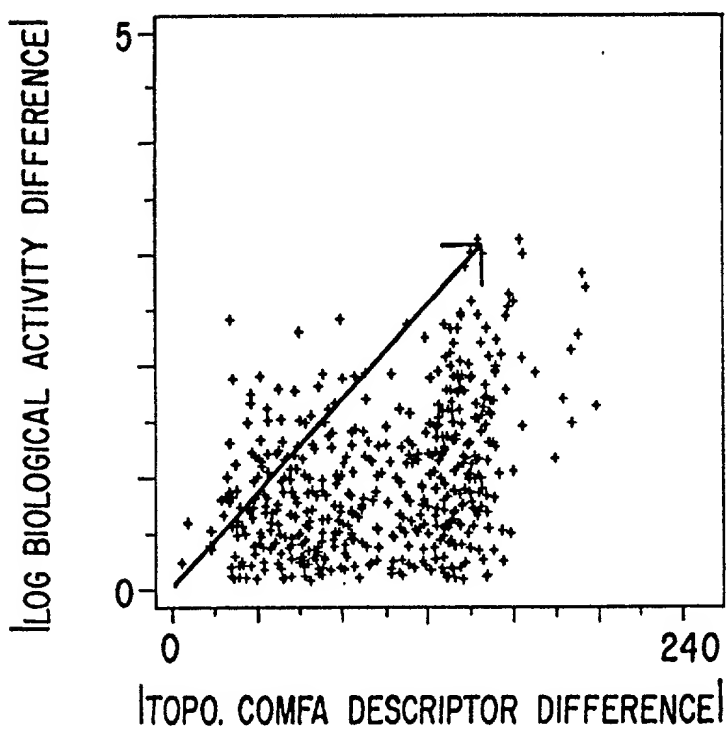


FIG.10(b)

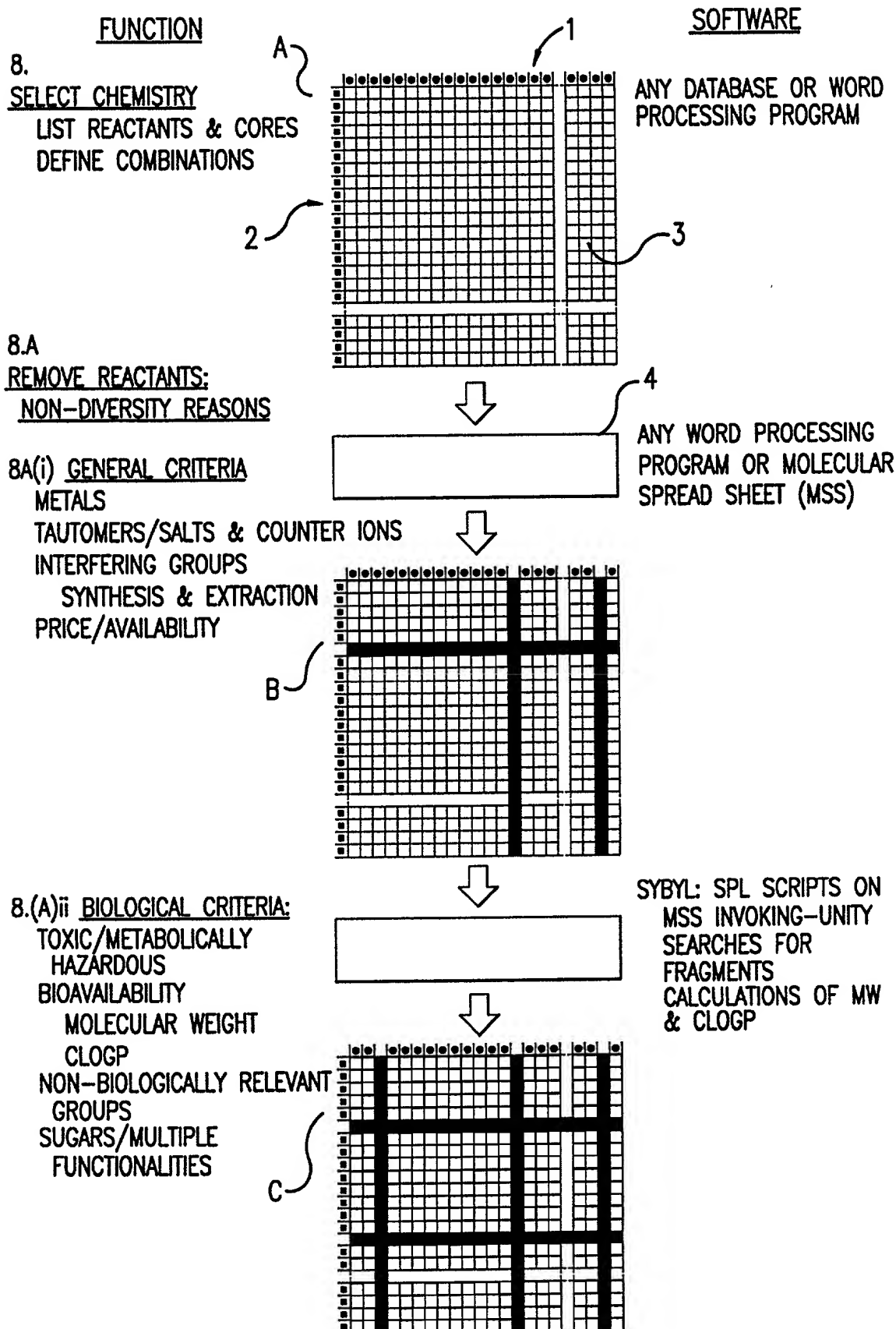


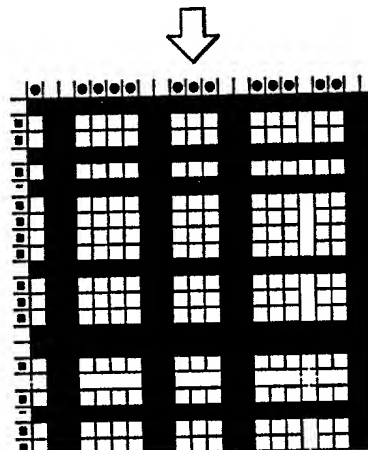
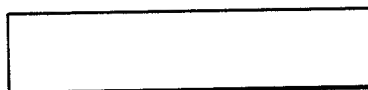
FIG.11(a)

8B

REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION  
 TOPOMERIC CONFORMER  
 ALIGNMENT  
 CoMFA FIELD GENERATION:  
 HYDROGEN BOND FIELD  
 GENERATION  
 ROTATABLE BOND FIELD  
 ATTENUATION  
 CALCULATE FIELD  
 DIFFERENCES  
 CLUSTER  
 REACTANT SELECTION FROM  
 EACH CLUSTER

D



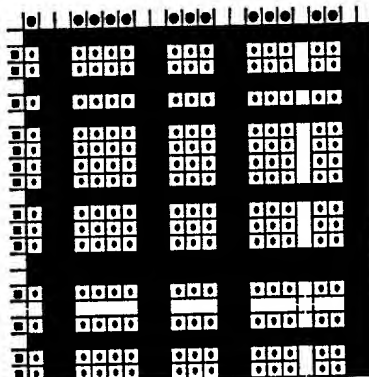
SYBYL: SELECTOR &  
 CONCORD 3.2.1  
 SPECIALIZED SOFTWARE:  
 APPENDIX "A"  
 (SYBYL: CoMFA  
 STERIC & MSS)

SYBYL: HIERCHICAL  
 CLUSTER - MSS  
 SYLBL: MSS

8C

COMBINE REACTANTS TO BUILD PRODUCTS

E



SYBYL: LEGION MSS

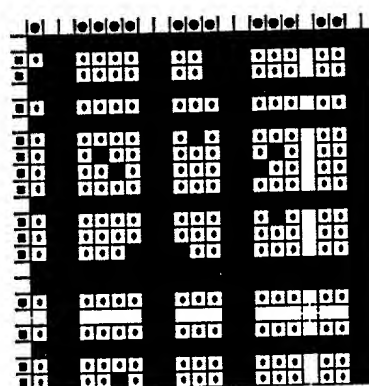
8D

REMOVE PRODUCTS:

NON-DIVERSITY REASONS

GENERAL CRITERIA:

F



SYBYL: SPL SCRIPTS  
 ON MSS

FIG.11(b)

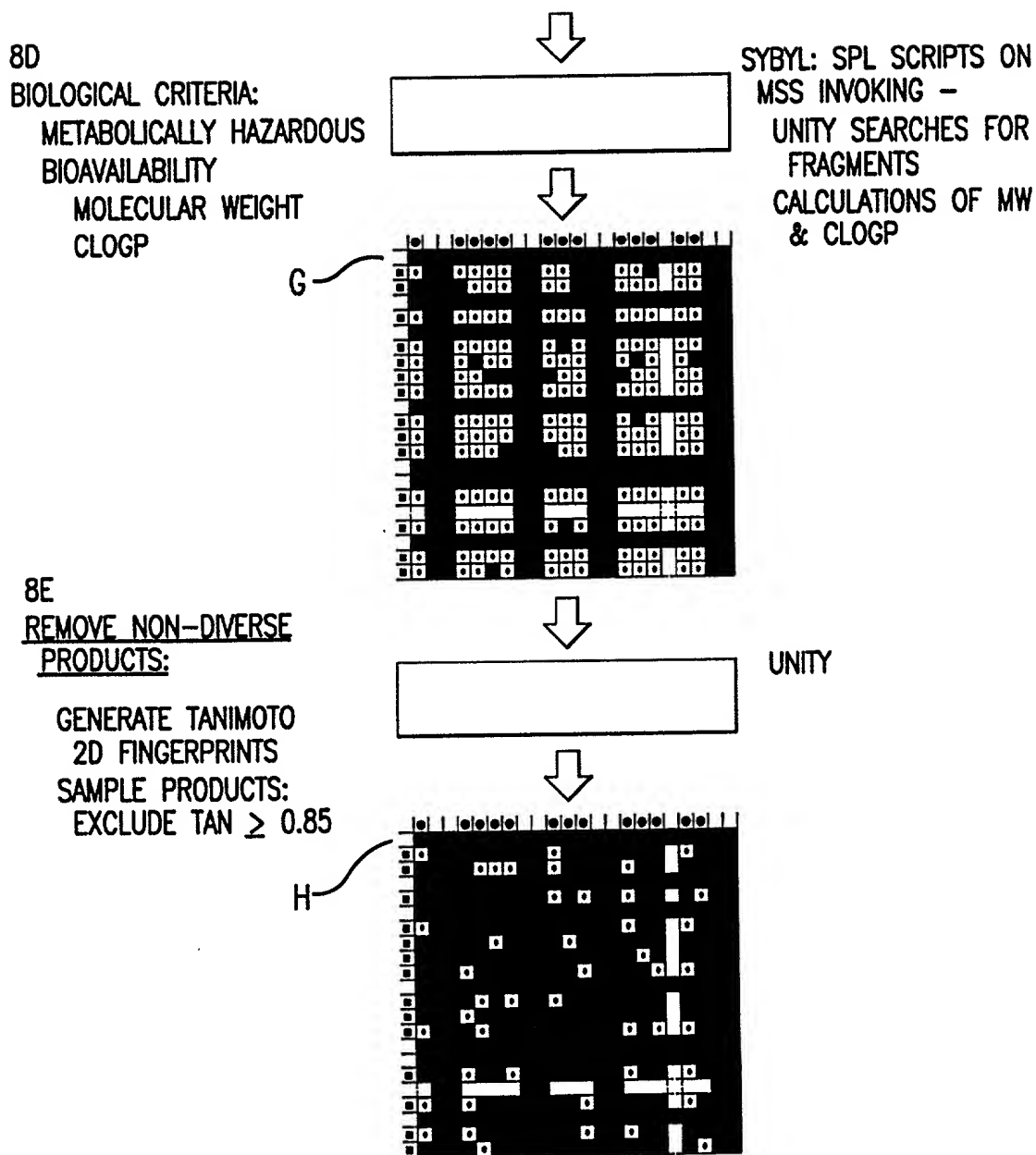


FIG.11(c)





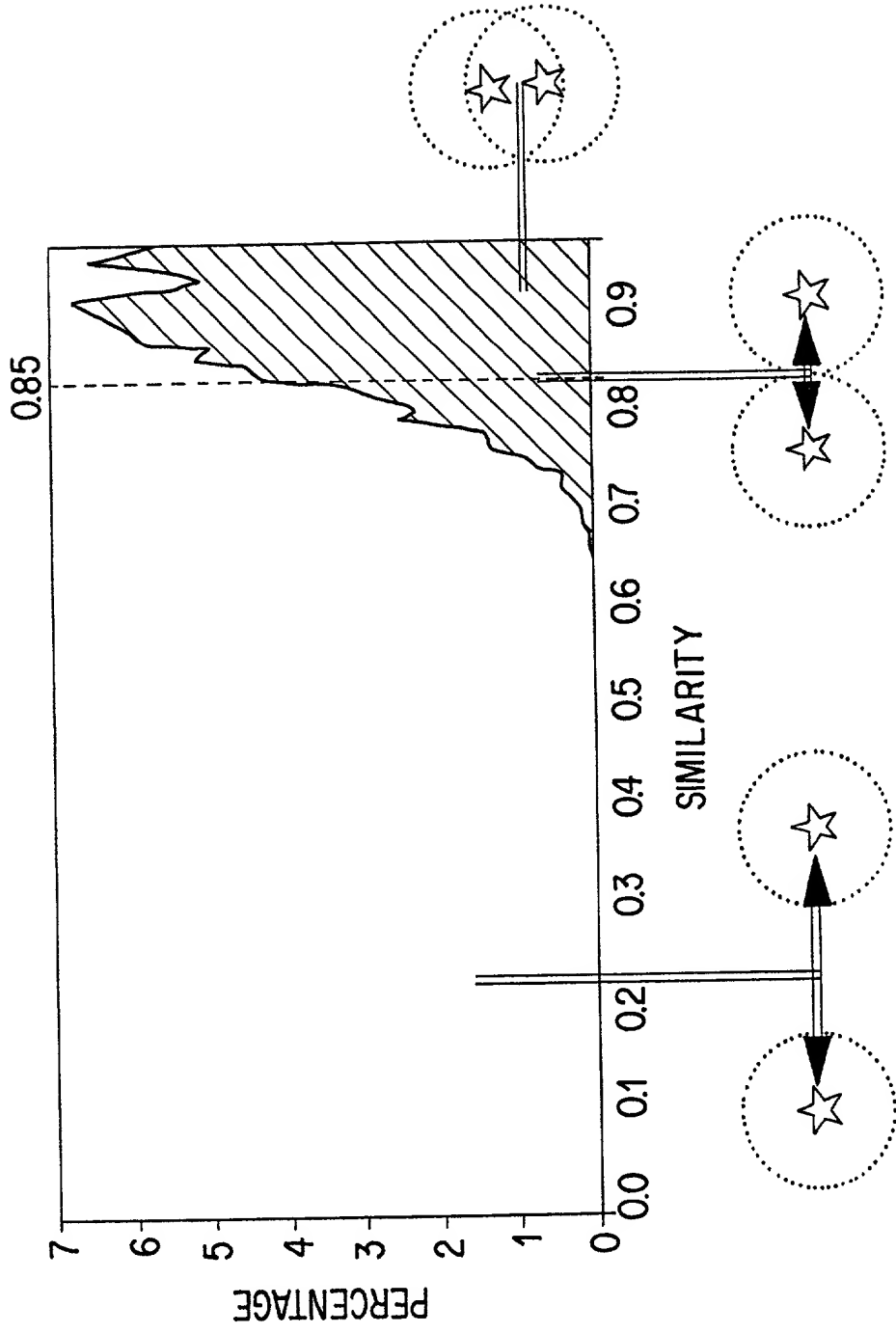


FIG. 13

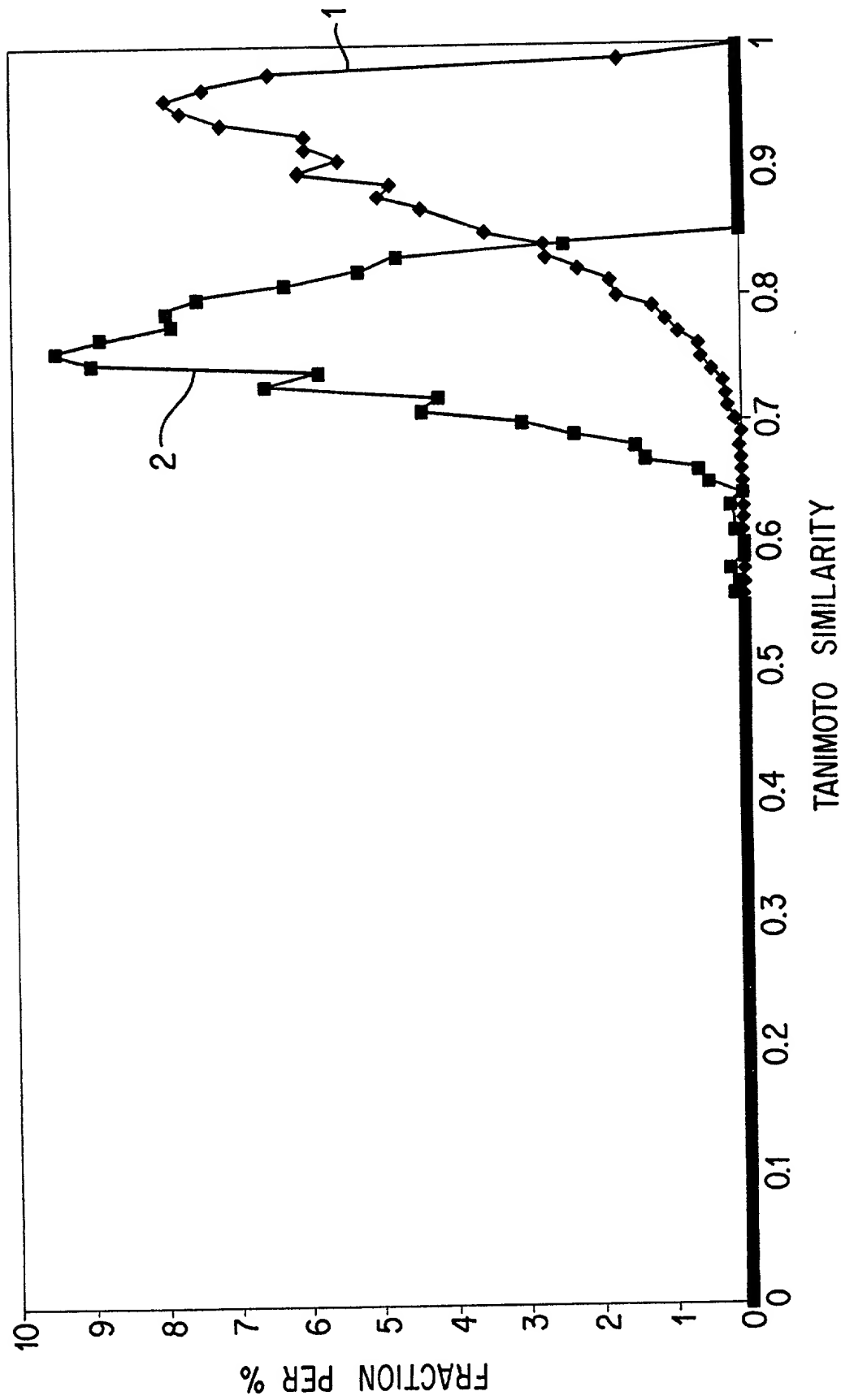


FIG. 14

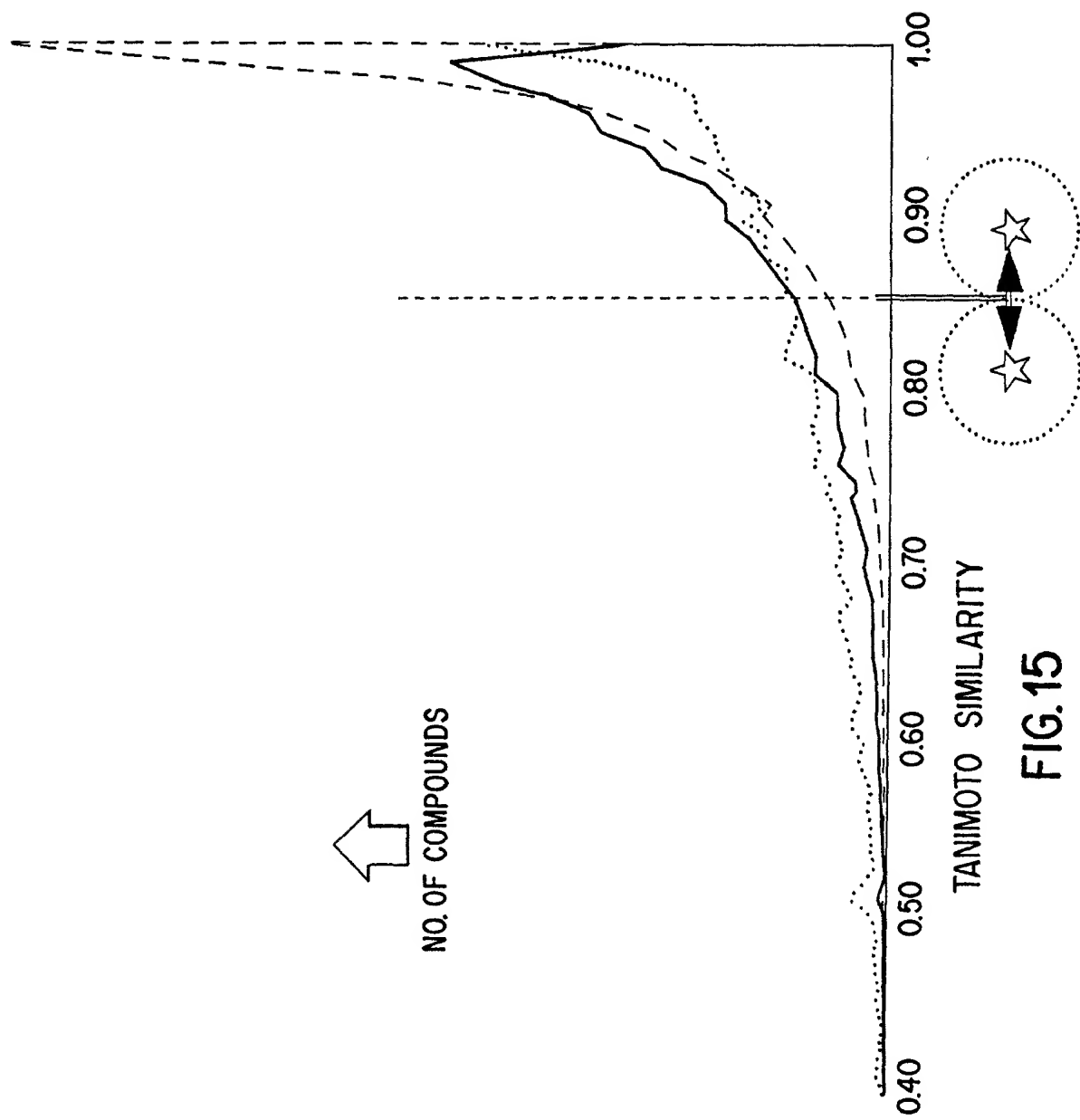


FIG.15